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Quantum Computation with Diatomic Bits in Optical Lattices

Chaohong Lee* and Elena A. Ostrovskaya
*Nonlinear Physics Centre and ARC Centre of Excellence for Quantum-Atom Optics,
Research School of Physical Sciences and Engineering,
Australian National University, Canberra ACT 0200,Australia*
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We propose a scheme for scalable and universal quantum computation using diatomic bits with conditional dipole-dipole interaction, trapped within an optical lattice. The qubit states are encoded by the scattering state and the bound heteronuclear molecular state of two ultracold atoms per site. The conditional dipole-dipole interaction appears between neighboring bits when they both occupy the molecular state. The realization of a universal set of quantum logic gates, which is composed of single-bit operations and a two-bit controlled-NOT gate, is presented. The readout method is also discussed.

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I. INTRODUCTION

Quantum computers based upon the principles of quantum superposition and entanglement are expected to provide more powerful computation ability than classical ones in the algorithms such as Shor's factoring [1] and Grover's searching [2]. Successful implementation of quantum information processing (QIP) would also have significant impact on many-body quantum entanglement [3], precision measurements [3, 4], and quantum communications [5]. To realize QIP, many schemes of quantum circuits have been proposed including those based on trapped ions [6], nuclear magnetic resonance [7], cavity quantum electrodynamics [8], linear optics [9], silicon based nuclear spins [10], quantum dots [11] and Josephson junctions [12]. Due to the long coherence times of the atomic hyperfine states and well-developed techniques for trapping and manipulating ultracold atoms in optical lattices [13], quantum computation schemes utilizing neutral atoms become particularly attractive [14, 15].

To realize a set of universal quantum logic gates with neutral atoms [16], the coupling between atomic bits must be strong enough for inducing entanglement. One of the suggested coupling mechanisms is the magnetic dipole-dipole interaction between single atoms trapped in different sites of spin-dependent optical lattices [17]. However, due to the very small magnetic dipole moment, one has to drive two atoms very close together by shifting the spin-dependent optical lattice potentials [17]. If the distance between two atomic bits is fixed and not very short, one has to induce sufficiently large electric dipole moments with auxiliary lasers [18] or other methods. Another possibility is to use neutral diatomic molecules with sufficiently large electric dipole moments [19]. However, the electric dipole-dipole interaction between molecules can not be controllably switched off and on. This lack of control requires additional refocusing procedures to eliminate the effects of the non-nearest-neighboring couplings [19].

Recently, applying the techniques of Raman transition, the single-state molecules from atomic Bose-Einstein condensate [20], state selective production of molecules in optical lattices [21] and optical production of ultracold heteronuclear molecules with large electric dipole moments [22] have been realized successfully. These experiments provide the potential possibility to perform quantum computation using diatomic bits with optically induced atom-molecular coherence. The atom-molecular coherence can also be induced by a magnetic field Feshbach resonance [23].

In this article, we suggest a new scheme for quantum computation based upon diatomic qubits with conditional electric dipole-dipole interactions. The qubits are realized by trapping neutral Bose-condensed atoms of two different species in an optical lattice and driving the system into a Mott insulator regime with only two atoms (and only one atom of each species) per site. Application of the well-developed technique of Raman transitions between the free atomic state and a bound molecular state at each lattice site [20] can ensure a well-defined two-state behaviour of the diatomic system at each site, and hence the qubit states can be encoded by these two states. For certain atomic species, the ground heteronuclear molecular state would naturally possess a large electric dipole moment. Due to the dipole-dipole interaction between dipolar molecular states in neighbouring wells, the two-bit phase gate can be naturally realized by free evolution. This dipole-dipole interaction is conditional upon neighbouring qubits occupuying molecular states, and can be controllably turned on and off. Combining the two-bit phase-gate with the single-bit Raman transitions, one can successfully implement a set of universal gates. The trapping and state selective production of molecules in optical lattices [21] enables an excellent scalability of the processor to a lot of qubits.

*E-mail: chl124@rsphysse.anu.edu.au; chleecn@gmail.com

II. QUANTUM COMPUTATION SCHEME

Let us consider two different species of Bose-condensed atoms loaded into a one-dimensional optical lattice with the potential $V(z) = V_0 \cos^2(kz)$, see Fig. 1 (a). If loaded adiabatically, the atoms will occupy only the lowest Bloch band. For sufficiently strong intensity of the laser that forms the optical lattice potential, the tight-binding limit is reached. Under these conditions, the system obeys the following Hamiltonian,

$$\begin{aligned} H = & -\sum_{\langle i,j\rangle}(t_a a_i^+ a_j + t_b b_i^+ b_j + t_c c_i^+ c_j + h.c.) \\ & + \sum_i \Omega_i (a_i^+ b_i^+ c_i + c_i^+ a_i b_i) + \sum_{\langle i,j\rangle} D_{ij} n_{ci} n_{cj} \\ & + \sum_\kappa^{a,b,c} \sum_i [U_{\kappa\kappa} n_{\kappa i}(n_{\kappa i} - 1)/2] \\ & + \sum_i (U_{ab} n_{ai} n_{bi} + U_{ac} n_{ai} n_{ci} + U_{bc} n_{bi} n_{ci}). \end{aligned} \tag{1}$$

Here, a_i^+ and b_i^+ (a_i and b_i) are bosonic creation (annihilation) operators for atoms on site i, c_i^+ (c_i) are corresponding operators for molecules on site i, and $n_{\kappa i} = \kappa_i^+ \kappa_i$ with $(\kappa = a, b, c)$ are particle numbers. The symbol $\langle i, j\rangle$ represents summing over the nearest-neighbors and $h.c.$ denotes the Hermitian conjugate terms. The first term describes the tunneling between neighboring sites with the tunneling strength t_κ. The second term corresponds to the coupling between atoms and molecules with Rabi frequencies Ω_i. The third term is the electric dipole-dipole interaction between molecules with the coefficients D_{ij} determined by the dipole moments and the lattice spacing. The last two terms describe the inter- and intra-component scattering with the coefficients $U_{\kappa\kappa'}$ determined by the s-wave scattering lengths.

A. Initialization

To initialize the processor, one can ramp up the potential depth after the two species of ultracold atoms are loaded into the optical lattice. For a sufficiently deep potential, the Mott insulator phase with $|n_{ai} = 1, n_{bi} = 1, n_{ci} = 0\rangle_F^G$ for every site can be easily obtained [24]. Here, F denotes the Fock states, and G denotes the ground states. Raman pulses can coherently couple the trapped atoms in the scattering state $|110\rangle_F^G$ and the diatomic heteronuclear molecular ste $|001\rangle_F^G$ at each site, which can therefore encode the qubit states $|0\rangle$ and $|1\rangle$, respectively. The Mott insulator state in the absence of coupling fields corresponds to the qubits state $|000...\rangle$.

B. Universal set of quantum logic gates

By properly choosing the atomic species, the heteronuclear molecules, such as RbCs and KRb [22], appear with very large electric dipole moments. By combining the techniques of coherent Raman transition and optimally controlled process (OCP) [25], the limit of Franck-Condon principle can be overcome. The single-bit operations (i.e., preparation of an arbitrary superposition of

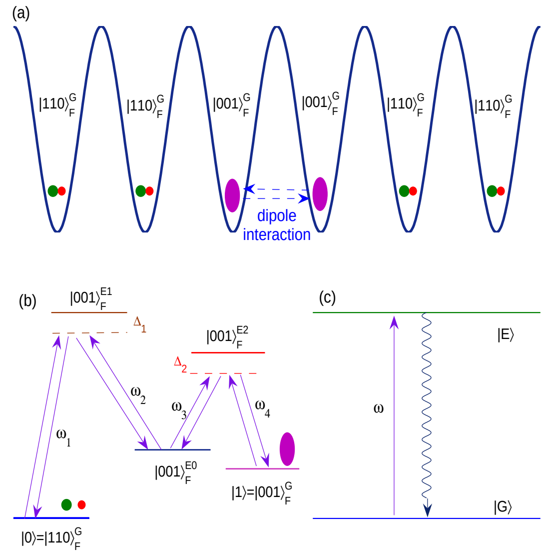

FIG. 1: (Color online) Scheme of quantum computation using diatomic qubits with conditional dipole-dipole interaction. (a) Diatomic qubits in one-dimensional optical lattices. The dipole-dipole interaction appears when neighboring bits occupy molecular states. (b) Single-bit operation with optimally controlled processes sandwiched Raman transition (see text). (c) Read-out with photon scattering (see text).

the atomic state $|110\rangle_F^G$ and the ground molecular state $|001\rangle_F^G$) can be realized with a Raman pulse sandwiched by two OCPs, see Fig. 1 (b). The first OCP transfers the ground molecular state to an excited one, the Raman pulse realizes the required superposition of the excited molecular state and the unbounded state of atoms, and then the second OCP transfers the excited molecular state back to the ground one.

The core task of quantum computation is to realize a set of universal quantum logic gates, such as single-bit operations combined with two-bit controlled-NOT gates [16]. As shown in Fig. 1 (b), the single-bit operations can be performed with optical stimulated Raman processes. A $R_y(\pi)$ pulse will transfer $|0\rangle$ (or $|1\rangle$) to $|1\rangle$ (or $|0\rangle$), and a $R_y(\pi/2)$ pulse will transfer $|0\rangle$ (or $|1\rangle$) to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ [or $\frac{1}{\sqrt{2}}(-|0\rangle + |1\rangle)$]. When all laser frequencies are detuned far from the transition frequencies to the excited molecular state, the excited molecular states will not be populated.

Because of the short distance (an order of a wavelength in an optical lattice) between neighboring bits and the same transition frequency for all bits, it is very difficult to selectively address a particular qubit by focusing the laser beams only on a particular site. Fortunately, similar to the well-developed techniques of gradient magnetic field in nuclear magnetic resonance, the transition frequencies for different bits can be distinguished by applying an ex-

ternal electric field [19],

$$\overrightarrow{E}_{ext} = \left(E_0 + z\frac{dE}{dz} \right) \overrightarrow{e}_x = (E_0 + gz)\overrightarrow{e}_x, \quad (2)$$

in the direction $\overrightarrow{e}_x$ perpendicular to the lattice direction $\overrightarrow{e}_z$, with a gradient g along the lattice direction $\overrightarrow{e}_z$. To dominate the system, the external electric field must satisfy the condition,

$$\mathrm{Min}(\left|\overrightarrow{E}_{ext}\right|) \gg \left|\overrightarrow{E^i}_{int}\right| = \left|\sum_{j\neq i} \frac{-\overrightarrow{d}_j n_{cj}}{4\pi\epsilon_0 |r(j-i)|^3}\right|. \quad (3)$$

Here, $\overrightarrow{E^i}_{int}$ is the internal electric field on site i created by the molecules in the neighboring site, $\overrightarrow{d}_j$ is the electric dipole moment for a single molecule on the $j-$th site, r is the distance between two nearest-neighboring sites, and the molecular occupation numbers n_{cj} are either 0 or 1. The difference between transition frequencies of nearest-neighbor bits,

$$\Delta\nu = \frac{\Delta E_{ext} d}{\hbar} = \frac{gdr}{\hbar}, \quad (4)$$

increases with the gradient. Thus, for a sufficiently large gradient, the selective addressing can be implemented by properly choosing frequencies of the laser fields. In Table I, we show $\Delta\nu$ for different diatomic bits XY (X = Li, Na, K and Rb; Y = Na, K, Rb and Cs) with $g = 1.0$ V/cm^2 and $r = 420$ nm corresponding to the optical lattices formed by a laser with wavelength $\lambda = 840$ nm [21]. All $\Delta\nu$ are in order of 100 Hz which are large enough to guarantee selective addressing a particular qubit without changing its neighbors.

Table I. Difference between transition frequencies of nearest-neighbor bits with $g = 1.0$ V/cm^2 and $r = 420$ nm. The related values for electric dipole moments are obtained from [26].

$\Delta v(XY)$	Na	K	Rb	Cs
Li	70.41 Hz	464.97 Hz	548.66 Hz	728.00 Hz
Na		365.33 Hz	442.38 Hz	611.10 Hz
K			85.02 Hz	255.07 Hz
Rb				167.39 Hz

To implement two-bit gates, one has to switch on the conditional dipole-dipole interaction between molecular states of neighboring bits,

$$D_{ij} = \frac{1}{4\pi\epsilon_0} \times \frac{\overrightarrow{d}_i \cdot \overrightarrow{d}_j}{|r(j-i)|^3}. \quad (5)$$

In this formula, we have assumed that both dipole moments are oriented along the external electric field. Because of the dominant strength of $\overrightarrow{E}_{ext}$, the electric dipole moments for the molecular ground state in different lattice sites have the same direction. In contrast to the quantum computation schemes utilizing polar molecules [19], the non-nearest-neighbor interactions can be switched off locally by transferring the non-nearest-neighbor bits into free atomic states. That is, the conditional dipole-dipole interaction $D_{ij} n_{ci} n_{cj}$ is switched off when the molecular occupation numbers n_{ci} or n_{cj} equal to zero. The controllability of these dipole-dipole interactions removes the need for the refocusing procedure [27] which eliminates the effects of non-nearest-neighbor interactions [7, 19].

Now let us analyze the realization of two-bit phase gates according to the dynamics governed by the Hamiltonian (1) with parameters in deeply insulating region of two different atoms or a molecule per site. Due to the dipole-dipole interaction only existing between molecular states, in free evolution the quantum logic state $|11\rangle$ will naturally acquire a phase shift. That is, an arbitrary two-bit state will be transformed as follows:

$$\begin{aligned} & C_{00}\,|00\rangle + C_{01}\,|01\rangle + C_{10}\,|10\rangle + C_{11}\,|11\rangle \\ & \longrightarrow C_{00}\,|00\rangle + C_{01}\,|01\rangle + C_{10}\,|10\rangle + C_{11}\exp(i\varphi)\,|11\rangle\,, \end{aligned} \quad (6)$$

with the phase shift,

$$\varphi = \frac{D_{12}t}{\hbar} = \frac{d_1 d_2 t}{4\pi\epsilon_0 \hbar r^3}, \quad (7)$$

determined by the coupling strength D_{12} and the evolution time t. Here the coefficients C_{ij} $(i, j = 0, 1)$ denote the probability amplitudes, and $d_{1,2}$ are electric dipole moments.

With the phase gate, it is easy to prepare four Bell states and construct a controlled-NOT gate [28]. The Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ can be prepared from the initialized state $|00\rangle$ (Mott insulating phase with two atoms per site) with the following steps: (i) a two-bit $\frac{\pi}{2}$ pulse, the initialized state is transferred into $\frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$; (ii) a π phase gate, the state freely evolves to $\frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + \exp(i\pi)|11\rangle)$; and (iii) a single-bit $\frac{\pi}{2}$ pulse for the first qubit. The other three Bell states can be obtained from this state by free evolution (π phase gate) or single-bit operation (single-bit π pulse). It is well known that the controlled-NOT gate can be constructed by two target-bit Hadamard gates sandwiching a π phase gate [28]. Usually, to simplify the pulse sequences, the first Hadamard gate is replaced with a single-bit $R_y(-\frac{\pi}{2})$ pulse and the second one is replaced with a single-bit $R_y(\frac{\pi}{2})$ pulse. This means that the time for a controlled-NOT gate equals the time for a π phase gate plus the time for a single-bit 2π pulse. Due to the very short time for a single-bit 2π pulse at large Rabi frequency, the total time for a controlled-NOT gate is dominated by the time for a π phase gate. By choosing the same parameters as for Table I, and ignoring the short times for single-bit operations, we can estimate the possible numbers of

controlled-NOT gates per second,

$$N = \frac{D_{12}}{\hbar\pi} = \frac{d_1 d_2}{4\pi^2\epsilon_0\hbar r^3}. \tag{8}$$

The values of N for different diatomic bits XY are shown in Table II. Most of the N values are of the order of 10^4, which guarantees that the system can successfully implement a lot of quantum logic gates before it loses quantum coherence.

Table II. Possible numbers of controlled-NOT gates per second.

$N(XY)$	Na	K	Rb	Cs
Li	1.14×10^3	4.99×10^4	6.94×10^4	1.22×10^5
Na		3.08×10^4	4.51×10^4	8.62×10^4
K			1.66×10^3	1.50×10^4
Rb				6.46×10^3

C. Readout

There are two different choices for reading out the final states. The first one is photon scattering which has been used to detect states of ion trap quantum computer [29]. The basic idea is illuminating the diatomic qubits with a circularly polarized laser beam tuned to the cycling transition from the ground state $|G\rangle$ of the selected particle (atom A, atom B, or molecule C) to the corresponding excited state $|E\rangle$, see Fig. 1 (c). If there are particles in $|G\rangle$, the photomultiplier will detect the scattered photons. Otherwise, there are no scattered photons. The second one is state-selective resonant ionization [19, 30]. In this method, one can apply a resonant laser pulse to selectively ionize the molecular ground state (qubit state $|1\rangle$) after rapidly switching off the external gradient electric field. Then the electrons and ions can be detected by imaging techniques.

D. Open problems

In real experiments, many practical factors must be taken into account. One is the strength of the optical lattice potential needed to keep the system in the Mott insulating phase with two different atoms or a heteronuclear molecule per site. In the further study, it would be interesting to analyze the details of quantum phase transitions to quantify the parameter region for the insulating phase, in particular, the effects of conditional dipole-dipole interaction and Raman coupling between atomic and molecular states. Another important factor is decoherence. As pointed out in previous studies [14], the decoherence from spontaneous emission can be avoided by choosing lasers far detuned from atomic transitions to form the optical lattices. In our model, we have also neglected the motional states localized in each lattice site. To avoid the coupling between motional excitation and gate operation, similar to the proposal by Jaksch et al. [15], one has to confine the qubits in deep Lamb-Dicke regimes to eliminate the significant momentum transfer to the qubits from the operational lasers. However, some vibrational and rotational molecular states and even some hyperfine states may be excited by the Raman processes. The effects of these excited states will bring a source of decoherence which is not easy to eliminate.

III. SUMMARY AND DISCUSSION

In conclusion, we have demonstrated the possibility of using diatomic bits with conditional dipole-dipole interaction to implement scalable and universal quantum computation. By trapping the ultracold diatomic bits within optical lattices, the system can be scaled to a large number of qubits. Combination of the coherent Raman transition between atomic and heteronuclear molecular states with the free evolution involving conditional dipole-dipole interaction makes the QIP based upon these diatomic qubits universal. Unlike the previous proposals for quantum computation in optical lattices, our proposal does not require relative shifting of the spin-dependent optical lattice potentials [14, 15], coupling to Rydberg states with large electric dipole moments [14, 18] or refocusing procedures to eliminate the effects of non-nearest-neighbor interaction [19]. We have also shown that the selective addressing of qubits can be realized by applying an external gradient electric field, and that the strength of dipole-dipole interactions guarantees the performance of a large number of quantum logic gates (in order of 10^4) per second.

Our analysis can also be applied to the case of two different kinds of Fermi atoms in optical lattices. For the system of Fermi atoms, due to the Pauli blocking, the s-wave scattering between Fermi atoms of the same kind is absent. That is, the Hamiltonian (1) has no terms containing U_{aa} or U_{bb}.

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